

Resorcinol monoacetate
102-29-4 | DTXSID6045901

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 36.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.04e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>(2-Chlorophenyl)urea</div> <div>Measured: 40.7</div> <div>Predicted: 51.3</div>	<div>Image not found</div> <div>1-Phenylurea</div> <div>Measured: 22.4</div> <div>Predicted: 34.2</div>	<div>Image not found</div> <div>Urea, (3-methylphenyl)-</div> <div>Measured: 36.3</div> <div>Predicted: 37.2</div>
<div>Image not found</div> <div>N-Methyl-N'-phenylurea</div> <div>Measured: 19.5</div> <div>Predicted: 29.8</div>	<div>Image not found</div> <div>3-Chlorophenylurea</div> <div>Measured: 102</div> <div>Predicted: 57.3</div>	